Plasma Facing Components E-Meeting 11/2/05

Plasma Edge/PMI Modeling

•J.N. Brooks (ANL) et al. “Beryllium (& tungsten) erosion/transport from ITER main chamber wall and divertor”

•E. Bringa (LLNL) “Summary and status of PFC atomistic simulations”

•A. Hassanein (ANL) et al. “ELMs mitigation by Noble Gas Injection”

•T. Evans (GA) et al. “Progress on 3-D heat transport modeling”

•T. Rognlien (LLNL) et al. “UEDGE ITER edge modeling”

•D. Ruzic (LLNL) et al. “Modeling and simulation work at UIUC”

"Beryllium (& tungsten) erosion/transport from ITER main chamber wall and divertor" J.N. Brooks ANL et al.

- As reported (PFC PPPL 5/05 meeting), we initiated analysis of ITER all-metal, mixed material (Be/W) PFC performance. (ANL, LLNL) (J.N. Brooks, J.P. Allain, M. Nieto, T. Rognlien). We computed beryllium sputtering from the first wall and transport to the divertor region and plasma, and rough T/Be codeposition magnitude—using code Package-OMEGA—for convective and non-convective plasma edge transport.

- **Latest work:**

  —New TRIM-SP calculations of oblique incidence D^+, T^+ on Be and W sputter yields.

  —Spatial resolution of wall-sputtered Be transport to/from outer vertical divertor target.

  —Tungsten-wall sputtering and transport.

  —Continued modeling/code-validation of PISCES mixed-material experiments. **(ANL, USCD)**

Package-OMEGA results*: ITER wall sputtering and transport

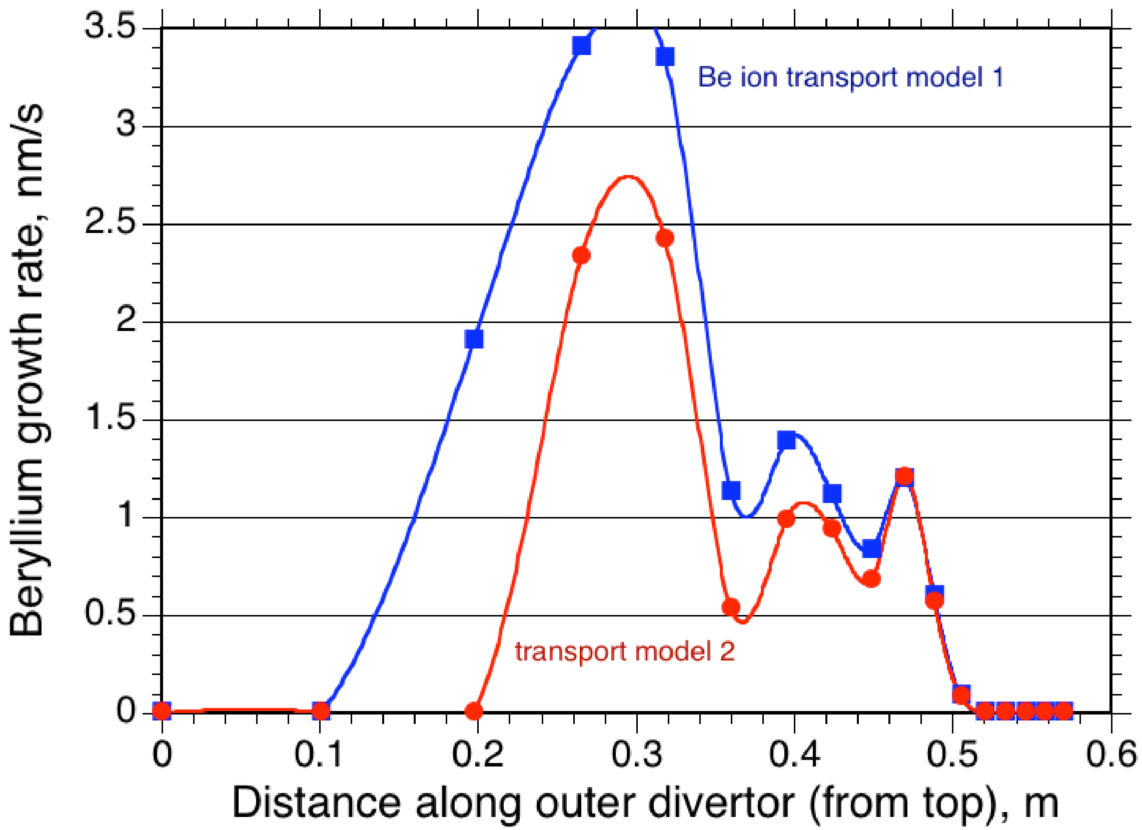
Plasma Case	Sputtered current **beryllium** s^{-1}	**tungsten** s^{-1}	Erosion rate** **beryllium** nm/s	**tungsten** nm/s
With convection	**3.9×10^{22}**	**$< 2 \times 10^{20}$**	**~ 1**	**< 0.01**
Diffusion only	**1.8×10^{21}**	**$< 2 \times 10^{20}$**	**0.02**	**< 0.002**

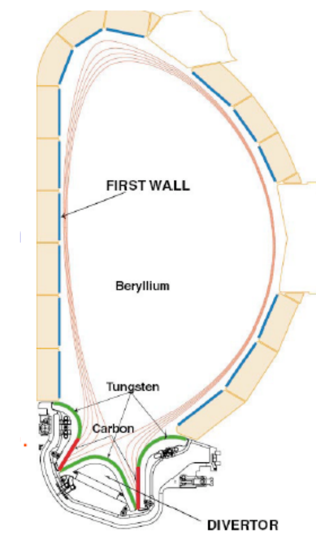
*preliminary impinging-particle energy model; next step = detailed energy/spatial distribution resolution.
** peak, w/o gas puffing

Be sputtering highly dependent on plasma case; tungsten sputtering very low

ITER wall-to-divertor beryllium transfer

(Be wall, W divertor) w/convection





Be growth on divertor generally modest. No growth on bottom/detached region (if also true for a carbon divertor, then Be transport would *not* suppress carbon chemical erosion).

ITER tungsten wall analysis: transport of sputtered tungsten

Plasma Case	Wall-sputtered fraction to divertor target	Wall-sputtered fraction to edge plasma*
With convection	**0**	**0**
Diffusion only	**0.002**	**0**

* 10,000 histories, prelim. results, no re-sputtering

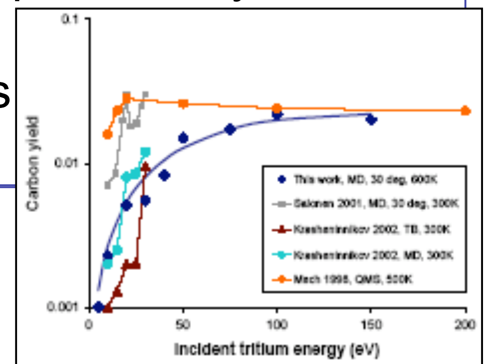
Plasma contamination by sputtering of a tungsten wall appears to be a non-issue.

Summary and status of PFC atomistic simulations

Goal: to simulate erosion rates using state-of the art AIREBO potential.
Problem: AIREBO has a number of advantages over REBO (used in previous studies) but, computationally, it costs significantly more.

Solution:

- Creating "realistic" amorphous carbon targets is extremely computationally expensive: mix REBO (bombardment) with AIREBO (relaxation) to obtain better targets. Synergy with LDRD-SI on edge plasmas
- use massive parallel computing at LLNL



Status:

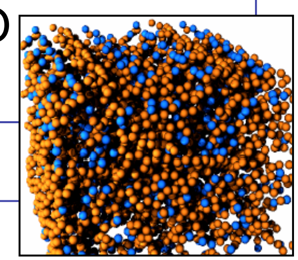
- Initial results (Phys. Scripta, Marian *et al*, in press) using melt-and-refreeze amorphous samples show:

i) difference between AIREBO and REBO is small at large energy (50 eV).
ii)relatively large differences between sputtering from different targets.

- Several new targets being created and tested using bombardment (LDRD-SI).
- Role of long-time chemical reactions being explored with ChemKin (LDRD-SI).

Next:

•Once targets are available, study difference between REBO and AIREBO bombardment at small energies (<20 eV).



Future: Explore H flux effects.

New: simulations of hydrocarbons with other species

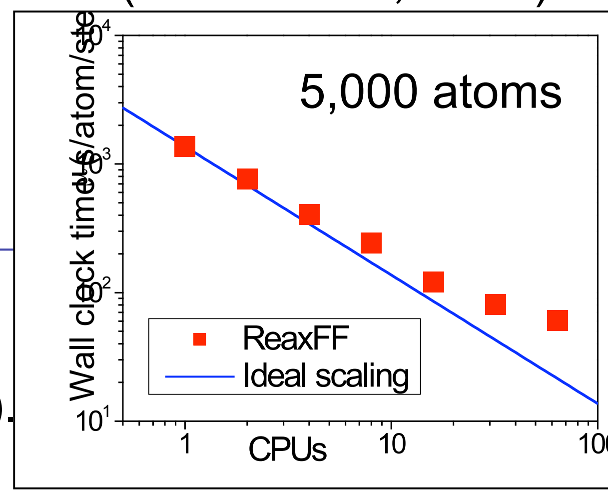
Goal: to perform realistic simulations of hydrocarbons and impurities like Li and Be.
Problem: REBO and AIREBO potentials include only C-H interactions.

Solution: use *ReaxFF* (A. van Duin, CalTech):

- Force: short-range + bond-order + dispersion + Coulomb (with variable charge).
- Chemistry well described (fitted to large dataset of reactions).
- Transferable parameters for C, H, Li, N, O, many more. Be in the near future (?)
- Problem until recently: extremely CPU intensive, and only a serial version available.
- Recent solution: *GRASP*, new parallel code developed by A. Thompson (SNL), including *ReaxFF*.

Status: *GRASP code successfully ported and tested* in MCR (2000 CPU's, LLNL)

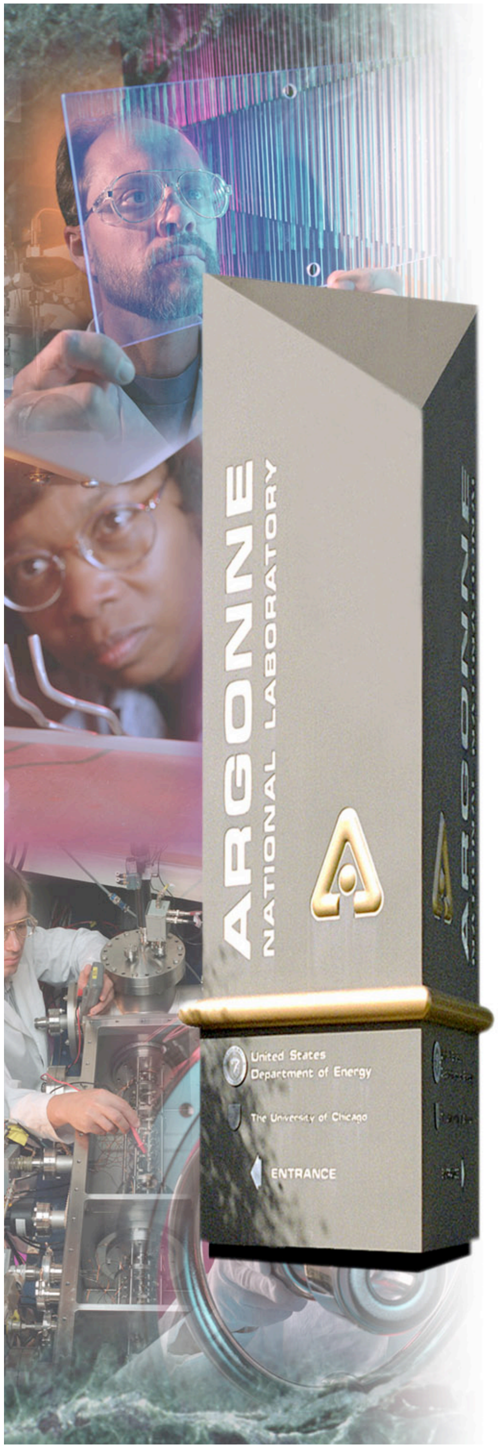
- Simulations runs for up to 5,000 atoms.
- ~60% parallel efficiency with 16 CPUs.
- CPU time/step ~10-20 times slower than REBO (comparable to full AIREBO).



Next:

- Sputtering runs:10 eV, 1,000 C:H atoms.
(expected: ~40,000 CPU hours for 2,000 cases in MCR).
- Repeat run with Li impurities.

Future: Run GRASP in BGL. Include Be or other metallic impurities.



ELMs mitigation by Noble Gas Injection, and Bubble Erosion in Liquid Lithium

I. Konkashbaev, Z. Insepov, A. Hassanein

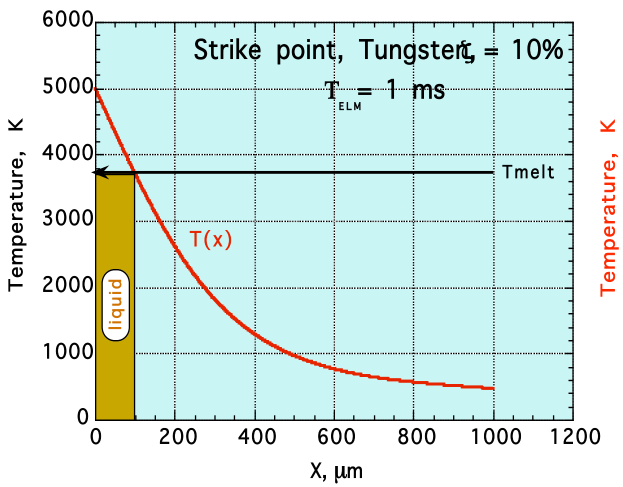
Presented at PFC Virtual Meeting
November 2, 2005

Argonne National Laboratory

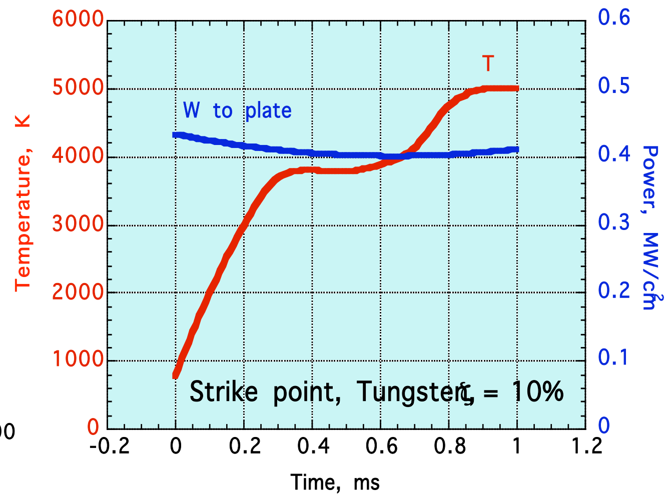
Office of Science
U.S. Department of Energy

A U.S. Department of Energy
Office of Science Laboratory
Operated by The University of Chicago

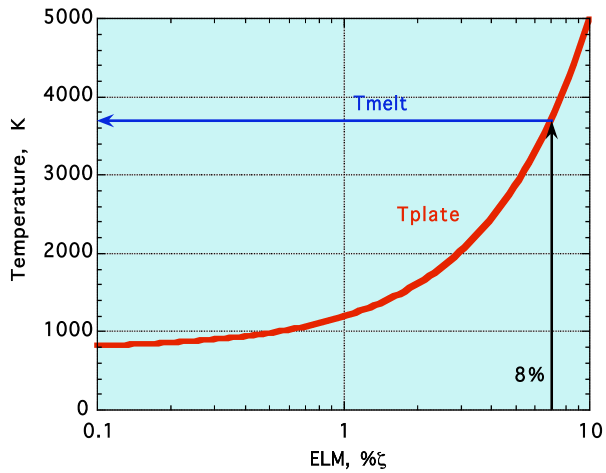
Response Of ITER Tungsten Divertor Plate Giant ELM, Q = 10%



Temperature at t =1 ms



Surface temperature as function of time.

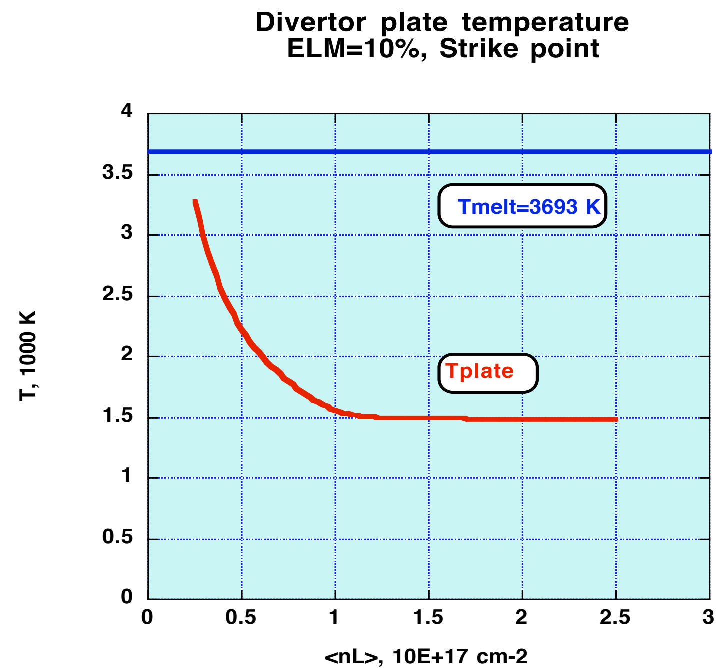


Surface temperature as function of ELM intensity

For low ELM intensity (<8%), surface temperature does not reach the melting temperature

Noble Gas Mitigation of ELMs

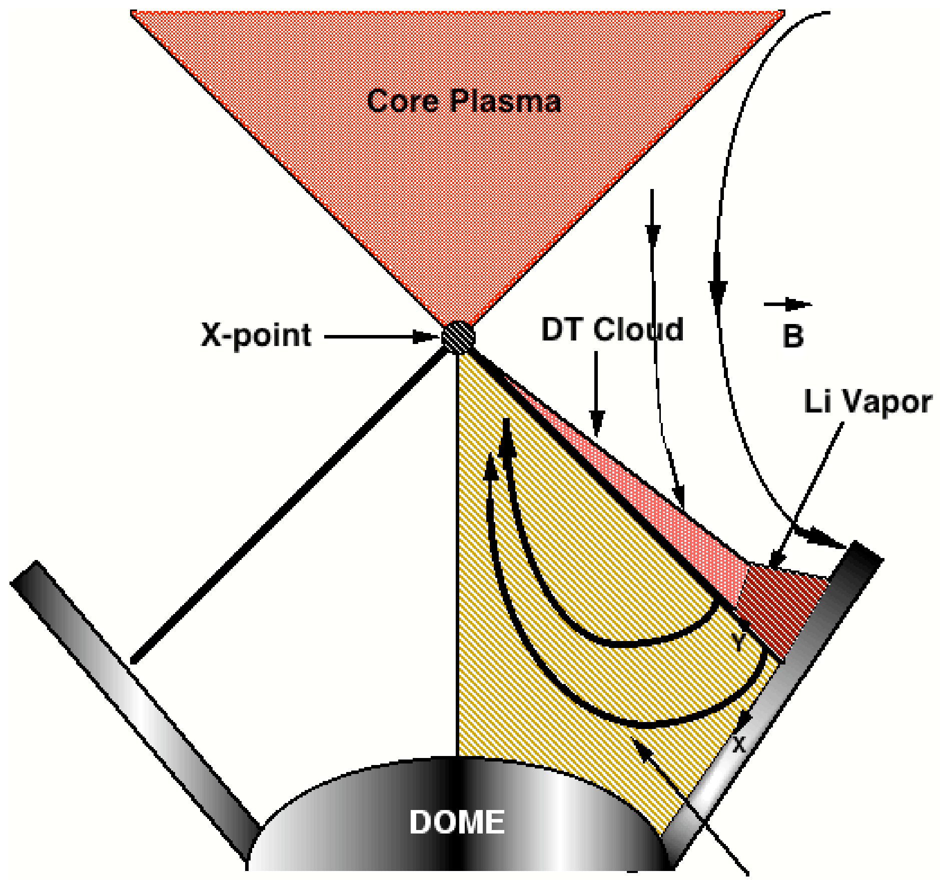
- ELM mitigation by a neon cloud puffed above the divertor surface is studied using the MHD HEIGHTS Package. We take into account full radiation transport of photons for both lines and continuum.
- The noble gas should have enough linear density, <nL>, to stop incoming particles, both ions and electrons, and reradiate a significant part of their energy.
- For a Giant ELM, the parameters of the Ne cloud are T≈ 4-5 eV, $\langle nL \rangle \approx 10^{17}$ cm^2, ($n \approx 10^{17}$ cm^{-3} , L ≈1 cm). Numerical simulations are made in detail to refine these estimates.
- Dependence of the tungsten surface temperature on the Ne cloud linear density shows that the shielding efficiency increases sharply for <nL> up to 10^{17} cm^{-2}, with asymptotic value of T=1500 K.



Core Plasma Contamination

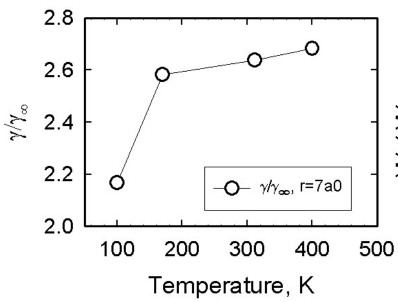
- Core plasma contamination during ELMs could be serious.

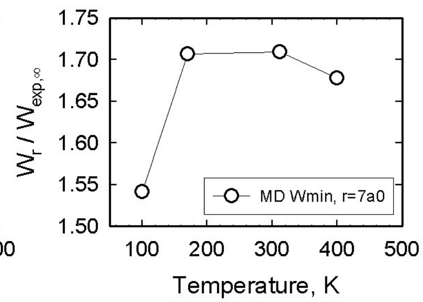
- There are two reasons for core contamination:
  - a) contamination during SOL reconstruction and
  - b) impurity diffusion along Private Flux Region (PFR)



Bubbles in liquid lithium

Temperature dependence of γ, W_{min}





$$W_{exp} = \frac{4\pi}{3} R_S^{\,3} \cdot \gamma_\infty$$

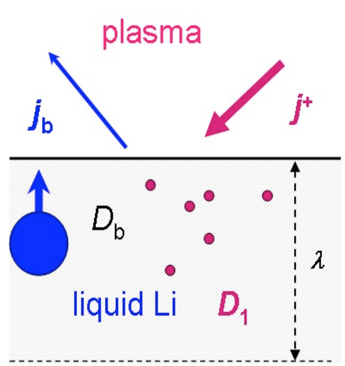
He bubble splashing model

$$Y_b = {\alpha j_b}/{j^+}, \quad C_b = C_1 B \exp\left[-{\Delta G^*}/{kT}\right] = C_1 B \cdot \varepsilon,$$

$$j_b = n_b^*(t) C_b \bar{v} = \frac{4}{3}\pi R_0^{\,3} \rho_b \exp\left[3\left(\frac{3\beta_D}{4}\cdot\frac{kT}{\gamma}\cdot j^+ \cdot t\right)\right]\cdot C_1 B \cdot \varepsilon \cdot \bar{v},$$

$$C_1 = j^+ \frac{\lambda}{D_1} \frac{1}{1 + n_b^*(t)\cdot\varepsilon}$$

- We have calculated ΔG^* for an empty cavity but it is unknown for a cavity filled with Helium.
- The parameter β_D is also unknown – need more work;
- We also need D_b – the bubble diffusion coefficient



$$\gamma = 0.4307 - 1.6262\times10^{-4}\times T(^\circ C)$$
$$\lambda = 10^{-6} m,\ t = 10^3\ s,\ D_1 = 10^{-9} m^2 s^{-1}$$

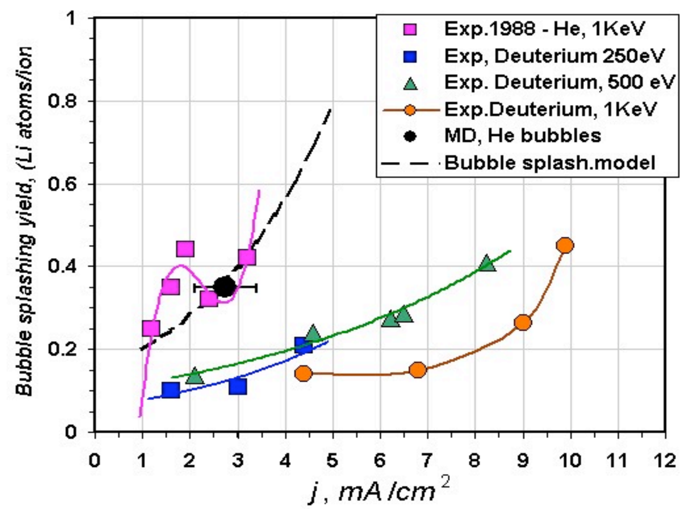
Low bubble concentration

If $n_b^*(t)\cdot\varepsilon << 1$,

$$Y_b = \alpha\,\rho_b \cdot \frac{4}{3}\pi R_0^{\,3} \exp\left[3\left(\frac{3\beta_D}{4}\cdot\frac{kT}{\gamma}\cdot j\cdot t\right)\right]\cdot const$$

For low fluxes (<1 mA/cm2), the bubble sputtering yield is negligibly small because the concentration of bubbles is small. For high ion fluxes, the bubble sputtering yield gives the main contribution to the total yield

Comparison with experiment



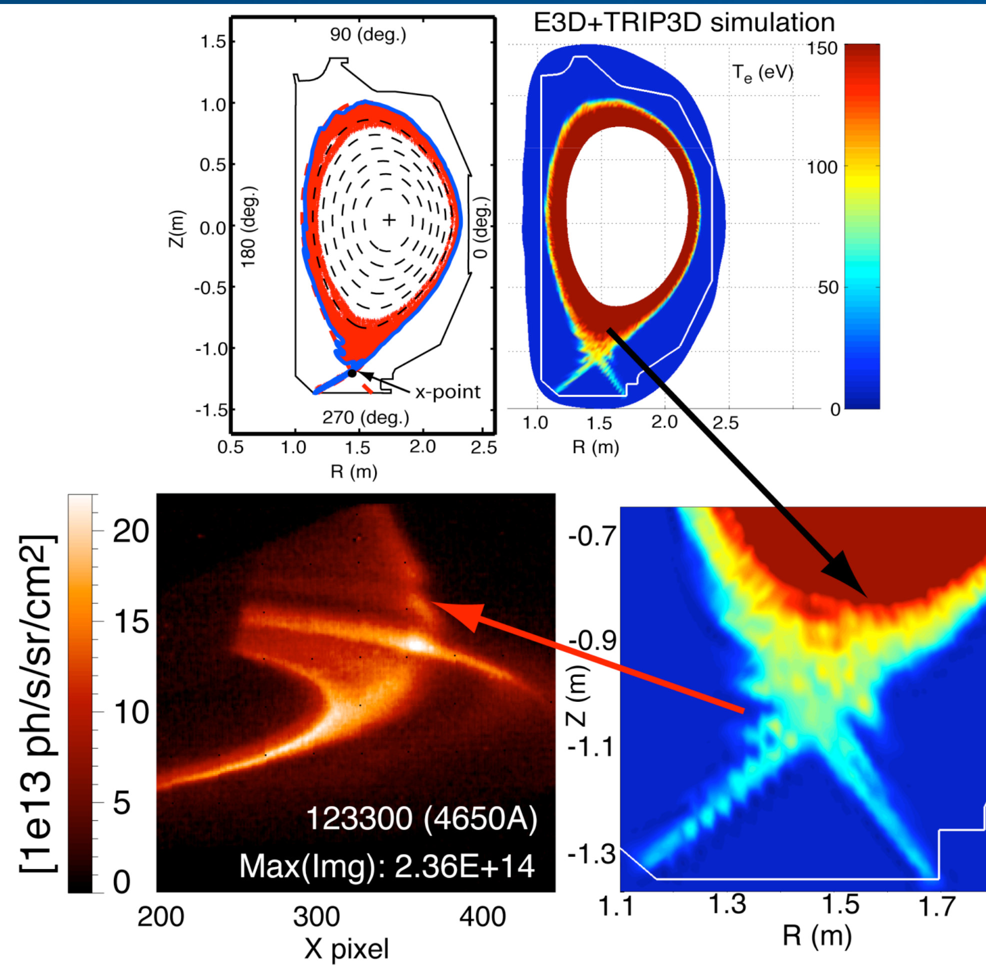
Progress on 3D heat transport modeling for pedestal and PMI control in burning tokamak plasmas

- TRIP3D field line integration code, developed at GA, calculates:
  - > Resonantly perturbed magnetic topology starting from axisymmetric Grad-Shafranov equilibria in DIII-D
    - Perturbations from non-axisymmetric field-errors and external control coils calculated with Biot-Savart algorithm
    - Field line trajectories/statistics and 3D seperatrix topology calculated
- E3D code, developed by MPI Greifswald team, calculates:
  - > non-axisymmetric heat transport using Monte Carlo fluid code
  - > 3D heat flux to plasma facing components and temperature distribution across outer plasma region (ψ_N>0.95)
- The TRIP3D and E3D codes have been coupled and used to model DIII-D pedestal, ELM and PMI control experiments in DIII-D
  - > Preliminary TRIP3D+E3D simulations have been compared with experimentally measured pedestal Te profiles and carbon emissions in the DIII-D divertor

E3D+TRIP3D energy transport modeling shows heating of non-axisymmetric (3D) x-point structure

- Non-axisymmetric x-point structures appear as a filament-like object in 2D images

- E3D+TRIP3D heat transport simulations reproduce temperature distribution consistent with observed X-point carbon emission

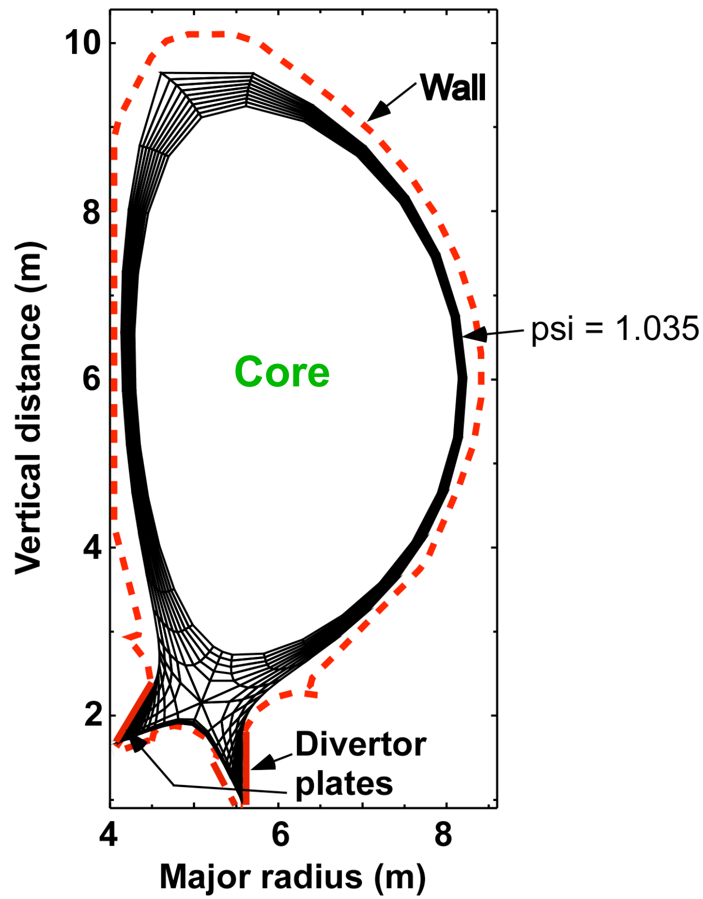


E3D+TRIP3D heat transport results:
A. Runov, R. Schneider (MPI Greifswald), S. Kasilov (Kharkov IPT), T. Evans (GA) and I. Joseph, R. Moyer (UCSD)

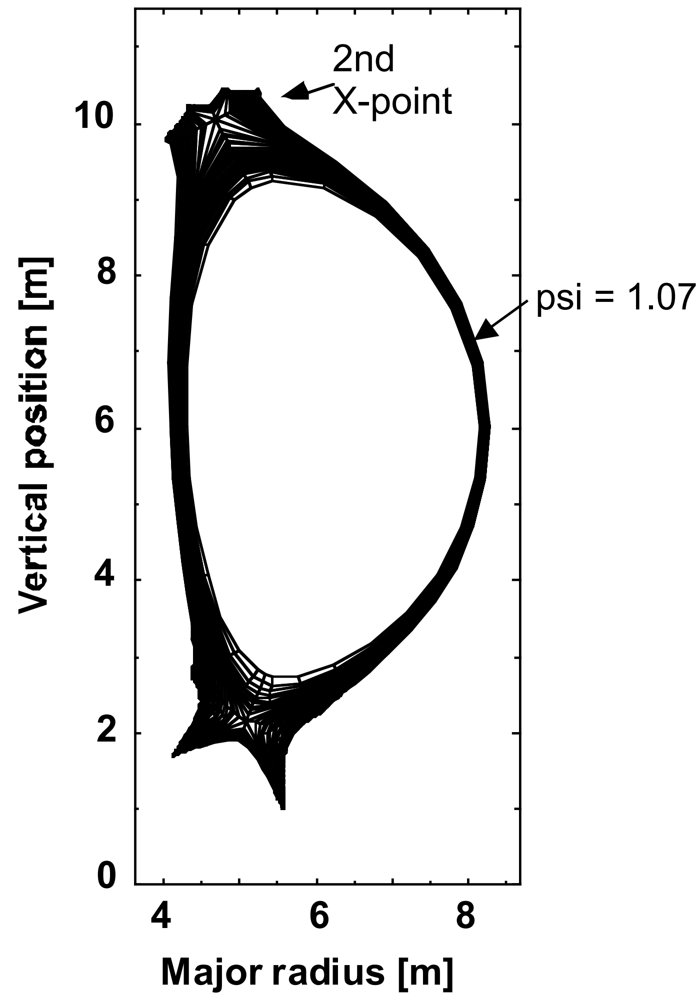
X-point carbon images:
M. Fenstermacher (LLNL), et al.,

The far SOL plasma in ITER is impacted by a 2nd upper X-point; we are working to model it

SOL region modeled by ITER team



Our first model doubles SOL width

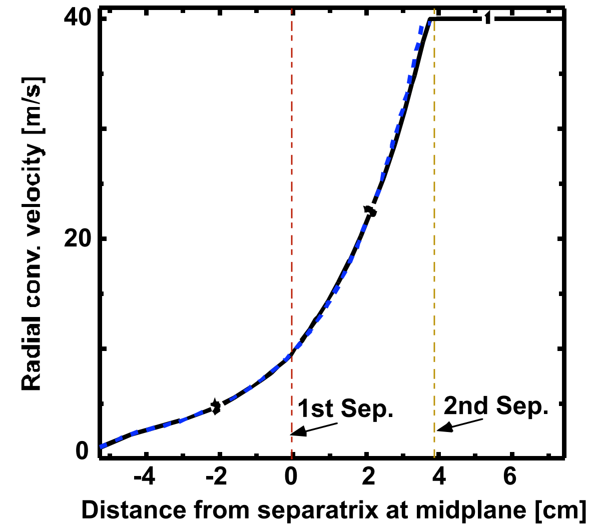


LLNL work by T. Rognlien, D. Bulmer, M. Rensink

We need a good far SOL model for plasma fluxes to wall and ionization of Be and W from diff. regions

- Main effect of outer SOL is reduced wall flux from n, T decay
- Larger wall distance attenuates neutrals (important for Be to carbon plates and hydrogen CX loss)
- Plan coupling to WBC's more detailed Be source

Blue - wall just before 2nd sep. (standard model)
Black - wall ~2x beyond 2nd sep.



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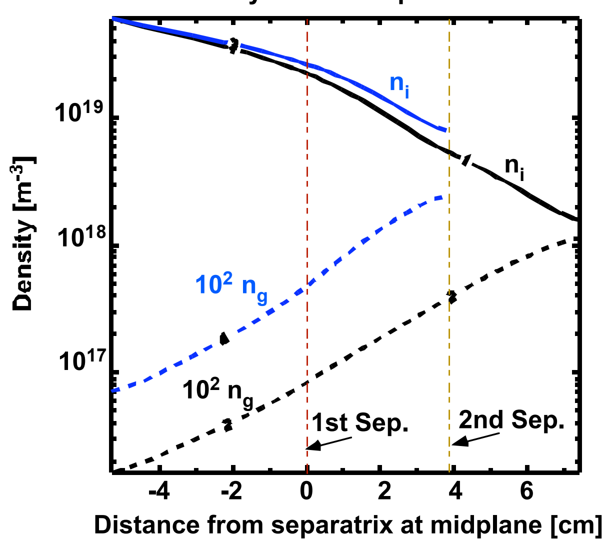
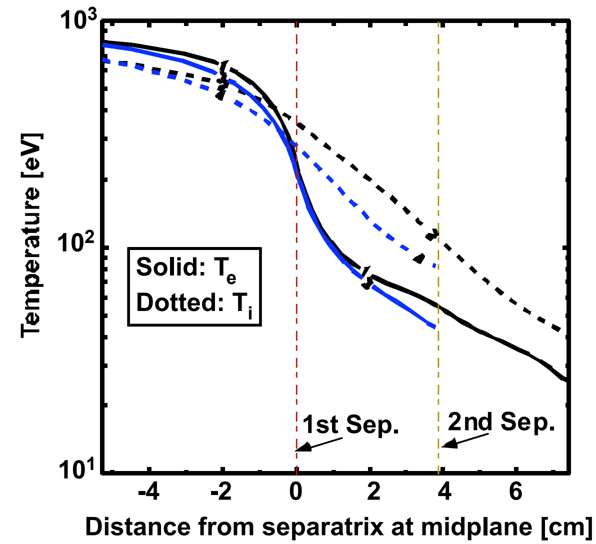
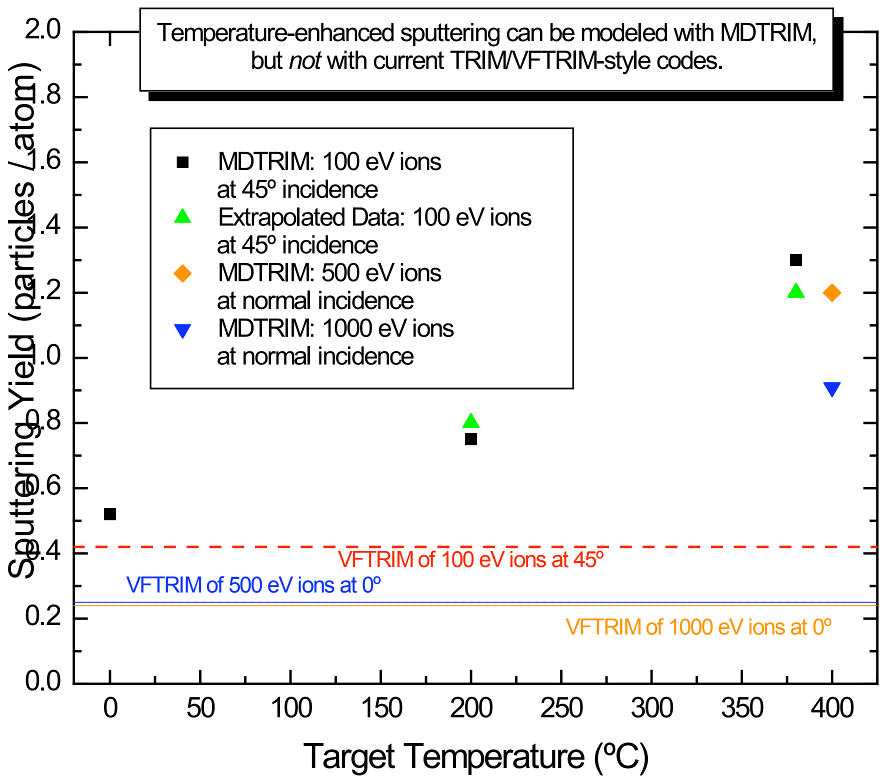




Modeling and simulation work at UIUC

Previous successes:

- MD molecular simulations of hydrocarbon-surface interactions for **C** fusion device surfaces including reflection, redeposition, and codeposition (w/ D, T).
- MD atomistic simulations of both deuterium and lithium bombardment of **solid** and **liquid** **lithium** with and without the presence of **D.**



Current and near-term focus:

- MDTRIM development to use kinematic relations of PKA creation and effective surface binding energy found from MD within the framework of VFTRIM to evaluate effects of temperature changes.
- Use of theoretical and empirical models in addition to MDTRIM simulations to improve understanding of temperature enhancement of liquid metal sputtering yields.
- In particular, the ion energy and ion mass dependence of the temperature enhanced sputtering yield

Longer-term:

- Modeling and simulations to support studies of ion bombardment of W-coated Be surfaces

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